 DOI 10.1515/jmbm-2012-0005 — J Mech Behav Mater 2013; 22(3-4): 81–88

Ilya A. Ovid'ko*

Plastic deformation mechanisms in nanocrystalline metallic materials

Abstract: This article discusses the experiments, computer simulations, and theoretical models addressing the conventional and specific mechanisms of plastic deformation in nanocrystalline metallic materials. Particular attention is devoted to the competition between lattice dislocation slip and specific deformation mechanisms mediated by grain boundaries as well as its sensitivity to grain size and other parameters of nanocrystalline metallic structures.

Keywords: deformation; grain boundaries; nanocrystalline metals.

***Corresponding author: Ilya A. Ovid'ko,** Institute of Problems of Mechanical Engineering, Russian Academy of Sciences, Bolshoj 61, Vas. Ostrov, St. Petersburg 199178, Russia; and Department of Mathematics and Mechanics, St. Petersburg State University, Universitetskii pr., 28, Staryi Petergof, St. Petersburg 198504, Russia, e-mail: ovidko@nano.ipme.ru

1 Introduction

Nanocrystalline materials have outstanding mechanical properties, thus giving rise to a wide range of new applications (see, e.g., reviews in [1–6] and the book, *Structural Nanocrystalline Materials: Fundamentals and Applications* [7]). For instance, nanocrystalline metallic materials often exhibit extremely high strength, superhardness, and good fatigue resistance desired for numerous technologies. At the same time, in most cases, ductility and fracture toughness of these materials are disappointingly low. In general, the mechanical properties of nanocrystalline metallic materials are significantly different from those of their coarse-grained counterparts. The difference is attributed to the effects of the specific structural peculiarities (such as nanoscopic grain sizes and large amounts of grain boundaries) on plastic flow and fracture mechanisms operating in nanocrystalline materials [1–7]. In particular, in parallel with conventional lattice slip, specific mechanisms of plastic deformation effectively come into play in nanocrystalline metals where the volume fraction of the interfacial phase is extremely high and grain size d does not exceed 100 nm. Such specific mechanisms include intergrain sliding, grain boundary diffusional creep (Coble creep), triple junction diffusional creep, rotational deformation, stress-driven migration of grain boundaries, nanodisturbance, and nanotwin deformation modes [1–7]. To enhance ductility and fracture toughness of nanocrystalline metals, a detailed knowledge on plastic deformation mechanisms operating at the nanoscale level in these materials is of the utmost importance. This article briefly presents and discusses current representations on plastic deformation mechanisms in nanocrystalline metallic materials and focuses on the competition between lattice dislocation slip and grain boundary deformation mechanisms as well as its sensitivity to grain size and other parameters of nanocrystalline metallic structures.

In general, nanocrystalline metallic materials can be divided into two categories: materials where lattice dislocation slip is dominant and those where grain boundary deformation mechanisms play the crucial role. More precisely, the slip of lattice dislocations – basic carriers of plastic flow in conventional coarse-grained polycrystals – is treated to be dominant in nanocrystalline materials with intermediate grains having the mean grain size d in the range from some critical value d_c (=10–30 nm) to 100 nm, where d_c is sensitive to structural and material parameters. In nanocrystalline materials with finest grains having the mean grain size $d<d_c$ (d_c=10–30 nm, depending on the material), grain boundary deformation mechanisms crucially contribute to plastic flow. At the same time, there are several deformation mechanisms that are weakly sensitive to grain size and that operate in nanocrystalline materials with both finest and intermediate grains. Below we will consider the specific peculiarities of lattice slip in nanocrystalline materials with intermediate grains (Section 2), grain boundary deformation mechanisms effectively operating in nanocrystalline materials with finest grains (Section 3), and deformation mechanisms weakly sensitive to grain size (Section 4). Concluding remarks are presented in Section 5.

2 Lattice dislocation slip and its specific peculiarities in nanocrystalline metallic materials with intermediate grains

The dominant deformation mechanism in conventional coarse-grained polycrystalline metals is the lattice dislocation slip occurring in large grain interiors (see, e.g., [8]). Its carriers are lattice dislocations generated and stored in the form of dislocation cells/subgrains in the grain interiors during plastic deformation. Grain boundaries serve as obstacles for movement of lattice dislocations, in which case they influence the level of the yield stress. This effect of grain boundaries in coarse-grained polycrystalline metals is described by the following classical Hall-Petch relationship between the yield stress τ and grain size d [9]:

$$\tau=\tau_0+kd^{-n}, \quad (1)$$

where τ_0 is the friction stress for movement of individual dislocations, k is a material constant parameter, and n=0.5. This relationship is conventionally attributed to the role of grain boundaries as stoppers of lattice dislocation pileups, and the yield stress τ is interpreted as the critical stress for movement of dislocation pileups (having lengths of around d) across grain boundaries [9].

At the same time, in most cases, the mechanical behavior of coarse-grained polycrystalline metals is crucially affected by evolution of lattice dislocations in grain interiors, but not grain boundaries. For instance, the deformation-induced storage of lattice dislocations in grain interiors in coarse-grained polycrystalline metals is responsible for the flow stress level and its evolution during plastic deformation. Commonly, the flow stress increases with rising plastic strain in polycrystals. This standard, strain-hardening behavior is exhibited by most coarse-grained polycrystalline metals with grain size d being larger than 1 μm.

With grain size reduction down to d_c, the lattice dislocation slip is still dominant. However, the lattice slip in nanocrystalline materials with intermediate grains shows its specific behavioral peculiarities due to both the nanoscale and the interface effects. First of all, the number of lattice dislocations composing a pileup in a nanoscale grain is small, and this factor modifies the classical Hall-Petch relationship [6, 10]. More precisely, when the grain size d is in the range from d_c to 100 nm, the yield stress is given by formula (1), with the exponent n being in the interval $0<n<0.5$ [6, 7].

Also, in contrast to the situation with conventional coarse-grained polycrystals, lattice dislocations are not intensively stored in grain interiors in ultrafine-grained metals (with grain size being in the range from 100 nm to 1 μm) and nanocrystalline metallic materials with intermediate grains. In these materials, the flow stress is crucially affected by the generation, storage, and annihilation of perfect and partial dislocations at grain boundaries [11] (Figure 1). The dislocation generation and storage at grain boundaries provide the strain hardening of a metallic material during plastic deformation. The dislocation annihilation at grain boundaries provides the strain softening (decrease in the flow stress with rising plastic strain) of a material during plastic deformation. Following [11], after some initial stage of deformation, the above competing factors reach equilibrium. That is, these factors cause a steady state in which the dislocation storage is completely compensated by the dislocation annihilation. The steady state is characterized by an approximately

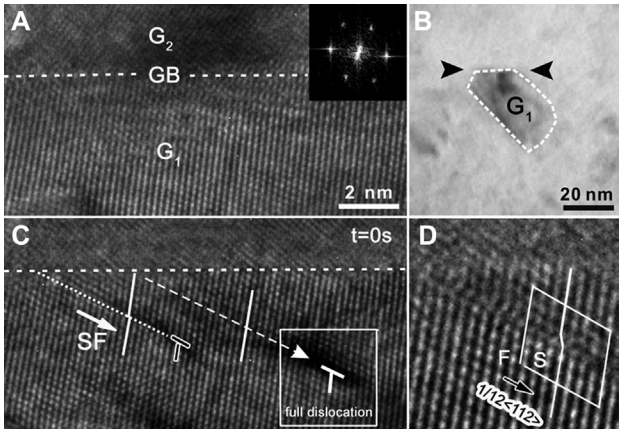

Figure 1 *In situ* transmission electron microscopy (TEM) observations of partial and full dislocations in nanocrystalline Ni. (A) A high-resolution TEM image of a grain (G_1) with no preexisting dislocation before tensile loading. The inset shows the fast Fourier transform pattern of G_1. The grain boundary between G_1 and its adjacent grain (G_2) is marked by a white dashed line. (B) Low-magnification image of the grain G_1 with the outlined boundary. Two arrows indicate the grain boundary between G_1 and G_2, as shown in (A). (C) After loading, a partial dislocation and a full dislocation, marked by black "T" and white "T," respectively, nucleated from the grain boundary and then propagated into the interior of G_1. The (111) slip planes are indicated by dashed white lines. The stacking fault (SF) left behind the partial dislocation is marked by the dotted-dashed line. (D) A magnified high-resolution TEM image of the partial dislocation during recovering. The stacking fault is indicated by a fold line. Reprinted from [12]. Copyright 2010, with permission from the American Institute of Physics.

constant flow stress, in which case strain hardening of the material during its plastic deformation is by practice absent. Due to the absence of strain hardening, nanocrystalline metallic materials with intermediate grains under tensile load are typically unstable relative to the necking [7, 11]. That is, they tend to show plastic strain instability, which suppresses their tensile ductility. As shown in a lot of experiments, this deformation behavior is typical for most ultrafine-grained materials and nanocrystalline materials with intermediate grains (see [7, 11] and references therein).

3 Plastic deformation mechanisms in nanocrystalline metallic materials with finest grains

In nanocrystalline metallic materials with finest grains, the lattice dislocation slip is very limited or even completely suppressed [1–7] because grain boundaries (whose amount is extremely large) stop gliding lattice dislocations. At the same time, alternative, grain boundary deformation mechanisms/modes such as intergrain sliding, Coble creep, triple junction diffusional creep, rotational deformation, stress-driven migration of grain boundaries, nanodisturbance, and nanotwin deformation modes are treated to effectively operate in nanocrystalline metals [1–7]. Crossover from the lattice slip to grain boundary deformation modes manifests itself, in particular, in the $\tau(d)$ dependence. More precisely, in the range of small grain sizes $d<d_c$, the $\tau(d)$ dependence in nanocrystalline materials exhibit either "inverse" Hall-Petch behavior (softening with reduction of grain size) or no "inverse" behavior (the yield stress saturates at grain size $d\leq 10$ nm) [6, 7].

Let us discuss grain boundary deformation mechanisms/modes. First, consider intergrain sliding, which often significantly or even dominantly contributes to plastic flow in nanocrystalline metallic materials with finest grains (see, e.g., [1–7, 13–15]). This deformation mode means a relative shear of neighboring grains that is localized in the boundary between the grains. As grain boundaries end at triple junctions, such junctions serve as natural geometric obstacles for intergrain sliding. In this situation, the unfinished plastic shear (or, in terms of grain boundary dislocations, the dislocation Burgers vector) associated with intergrain sliding is accumulated at triple junctions, which thereby serve as stress sources.

There are several ways for the accommodation of the unfinished plastic shear at triple junctions in nanocrystalline materials: the lattice dislocation emission from triple junctions (Figure 2), diffusional accommodation, rotational deformation, and void formation (Figure 2C) [12, 16–22]. The lattice dislocation emission from triple junctions seems to be a rather widespread process in various nanocrystalline materials (see the discussion in [20, 21]). Intergrain sliding accommodated by the dislocation emission process is characterized by creep strain rate [20, 21]:

$$\dot{\varepsilon}_{is}\approx 9bD_{gb}\cdot d^{-3}[\exp(2M\tau b^3/k_BT)-1], \quad (2)$$

where b denotes the lattice parameter, τ is the applied shear stress, M is the stress concentration factor (at triple

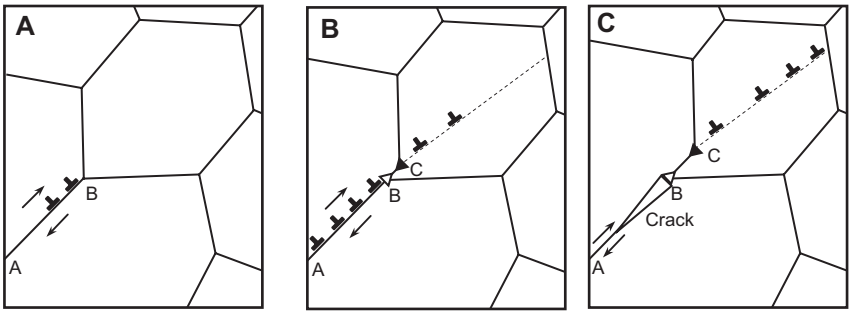

Figure 2 Intergrain sliding and its accommodation through lattice dislocation emission from triple junctions in a nanocrystalline solid. (A) Intergrain sliding (schematically marked by arrows) occurs through movement of grain boundary dislocations along grain boundary AB. Grain boundary dislocations are accumulated near triple junction B. (B) Grain boundary dislocations transform into lattice dislocations that are emitted from grain boundary junction C and glide within grain I. These processes are accompanied by formation of dipole of wedge disclinations (full and open triangles) B and C. (C) The distance between wedge disclinations B and C increases due to intergrain sliding. A nanocrack nucleates in the stress filed of the dipole of wedge disclinations B and C.

junction), k_B is the Boltzmann constant, and T is the absolute temperature.

Besides, intergrain sliding produces dipoles of wedge disclinations – defects associated with crystal lattice orientation incompatibilities – at and near triple junctions (Figure 2) [23]. [More precisely, a wedge disclination represents a rotational line defect located at either a grain boundary or a triple junction and characterized by the disclination strength, the rotational misfit [24]. For instance, a wedge disclination at a tilt grain boundary is the line dividing the grain boundary fragments with different tilt misorientation angles, whose difference is the disclination strength. A wedge disclination exists at a triple junction of tilt boundaries if the sum of tilt misorientation angles of these boundaries is non-zero [24]. The non-zero sum (angle gap) serves as the disclination strength.] Figure 2 schematically shows the formation of wedge disclination dipoles due to intergrain sliding in a nanocrystalline specimen (for more details, see [23]). Wedge disclination dipoles appearing in nanocrystalline metallic materials during intergrain sliding create very pronounced strain hardening, and this factor can significantly influence ductility of such materials [23].

Now let us briefly discuss diffusional creep modes operating in nanocrystalline metallic materials with the finest grains. The diffusion coefficient D_{tj} along triple junctions is much larger than the grain boundary diffusion coefficient D_{gb} [25], which, in its turn, is several orders larger than the bulk diffusion coefficient D_{bulk} [26]. Also, the volume fractions occupied by the triple junctions and grain boundaries rapidly increase (at the expense of the volume fraction occupied by grain interiors) with a decrease in grain size d in nanocrystalline materials. In these circumstances, the contributions of Coble creep and triple junction diffusional creep are enhanced with decreasing the grain size d [2, 6] more rapidly than that of the Nabarro-Herring creep (bulk diffusional creep). This tendency is reflected in the following grain size dependences of the plastic strain rates $\dot{\varepsilon}_{bulk}$, $\dot{\varepsilon}_{gb}$, and $\dot{\varepsilon}_{tj}$, which correspond to the Nabarro-Herring creep, Coble creep, and triple junction diffusional creep, respectively,

$$\dot{\varepsilon}_{bulk} \propto D_{bulk} \cdot d^{-2}\sigma, \qquad \dot{\varepsilon}_{gb} \propto D_{gb} \cdot d^{-3}\sigma, \qquad \dot{\varepsilon}_{tj} \propto D_{tj} \cdot d^{-4}\sigma \tag{3}$$

where σ is the applied tensile stress. As diffusional mass transfer is enhanced with increasing temperature, grain boundary and triple junction diffusional creep modes are capable of significantly contributing to plastic flow in nanocrystalline metallic materials with finest grains at intermediate and high temperatures [2, 6].

Rotational deformation in coarse-grained and nanocrystalline solids is defined as plastic deformation accompanied by crystal lattice rotations within grains [7, 24]. Rotational deformation is commonly carried by moving dipoles of grain boundary wedge disclinations [24]. Disclination dipole movement in coarse-grained polycrystals occurs through rearrangement of lattice dislocations in grain interiors [24]. In nanocrystalline metallic materials where the preexistence of lattice dislocations in grain interiors is very limited, rotational deformation occurs through (i) emission of lattice dislocations from grain boundaries and their absorption at opposite grain boundaries [27]; (ii) correlated generation and evolution of nanodisturbances (nanoscale areas where ideal plastic shear occurs) (Figure 3) [28]; and (iii) slip and climb of grain boundary dislocations [29]. In the latter case, the rotational deformation can be effectively initiated by the preceding intergrain sliding and serve as its accommodating mechanism [22]. The representations on rotational deformation are well supported by experimental observations of crystal lattice rotations within the grains in deformed nanocrystalline metallic materials [30–33].

4 Plastic deformation mechanisms operative in nanocrystalline metallic materials with finest and intermediate grains

Stress-driven migration of grain boundaries is capable of effectively contributing to plastic flow in nanocrystalline materials with fine and intermediate grains as well as ultrafine-grained metals. The pioneering experiments [34, 35] and other experimental works [36–38] in this area have demonstrated that stress-driven grain growth occurs during plastic deformation in ultrafine-grained and nanocrystalline metals and alloys at room [34–38] and cryogenic [36] temperatures. Computer simulations [39, 40] have demonstrated that low-temperature stress-induced grain growth in nanocrystalline metals is athermal. Its basic mechanisms in the simulations [39, 40] are found to be stress-induced migration of grain boundaries and their triple junctions (Figure 4), intergrain sliding, grain rotation, and coalescence. Also, stress-induced GB migration have been described theoretically as a specific deformation mode in nanocrystalline materials, using dislocation-disclination models [41–44]. These models predict the existence of critical values of the stress for migration of GBs. For

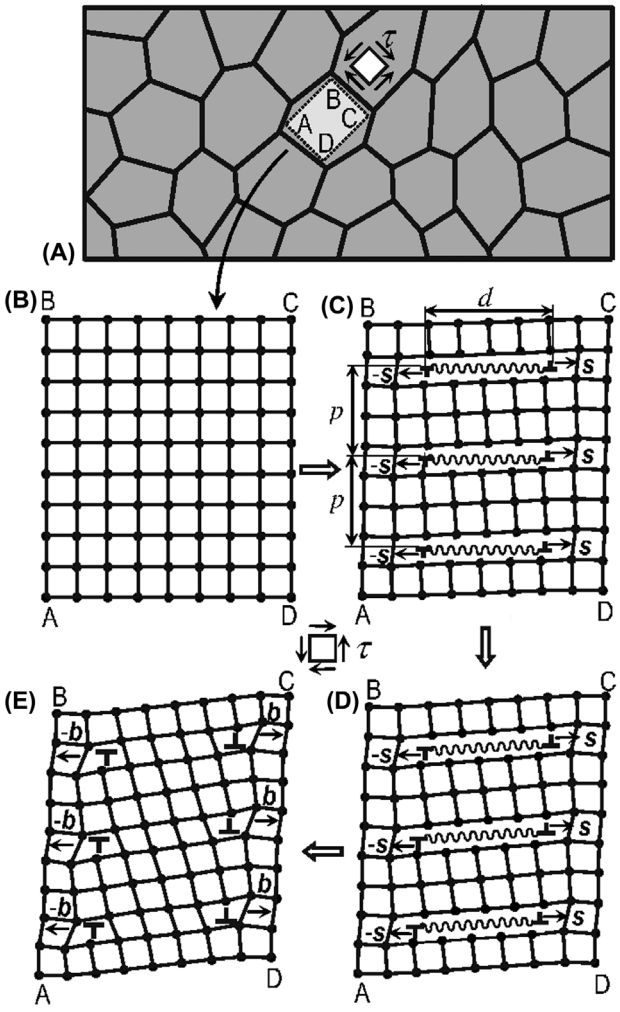

Figure 3 Nanoscale rotational deformation in nanocrystalline solid.
(A) Two-dimensional general view on nanocrystalline specimen. (B)–(E) Two-dimensional view on nanoscale rotational deformation in a crystallographic plane of a grain with a cubic crystalline lattice. (B) Initial state of a nanoscale grain. (C) A wall of nanodisturbances is generated. Each nanodisturbance consists of a dipole of noncrystallographic dislocations with tiny Burgers vectors ±s. Generalized stacking faults (wavy lines) are formed between the dislocations composing the nanodisturbances. (D) The Burgers vector magnitude *s* (characterizing the nanodisturbances) gradually increases, and generalized stacking faults evolve in parallel with growth of *s*. (E) The non-crystallographic dislocations transform into conventional perfect dislocations (when *s* reaches the Burgers vector magnitude *b* of a perfect dislocation) and generalized stacking faults disappear. Reprinted from [28]. Copyright 2011, with permission from the American Institute of Physics.

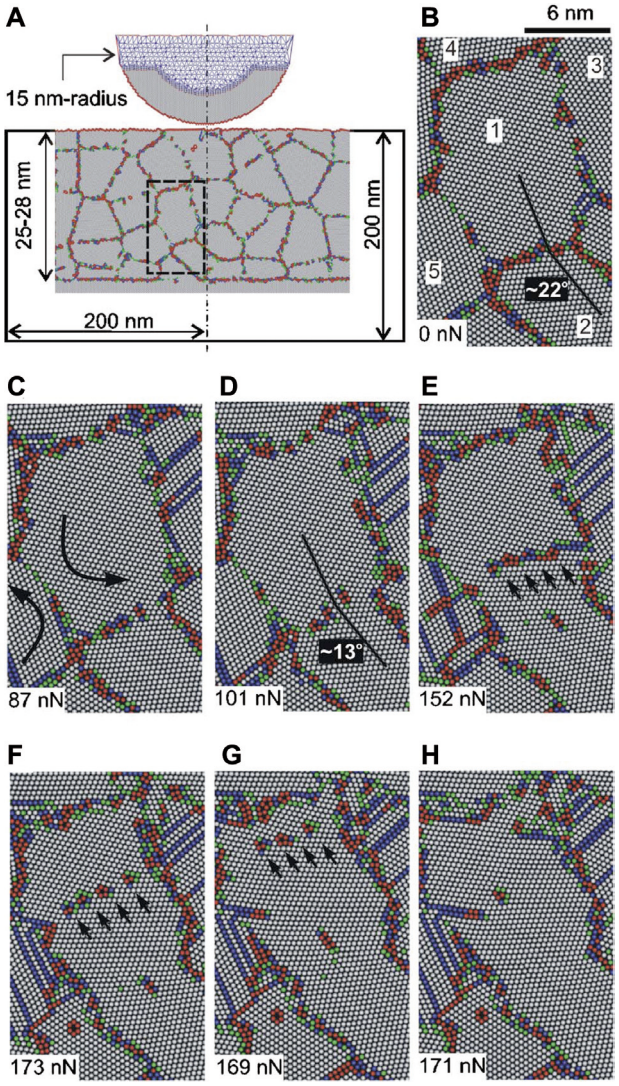

Figure 4 Deformation of a representative grain cluster in the prolongation of a shear band in the 7-nm grain size Al film.
(A) Contact zone before indentation. Dimensions and location of the fully refined atomistic region are indicated with respect to the atomistically informed finite element domain (not to scale). Dashed area shows the location of the grain cluster. (B)–(D) Rotation of grain 1. (E)–(H) Motion of the boundary separating grains 1 and 2. The applied contact force is indicated in the lower left corner of the images. Reprinted from [39]. Copyright 2006, with permission from the American Institute of Physics.

instance, the critical stress τ_{cr} needed to initiate migration of a tilt boundary with both the length d' and tilt angle ω is given as [41]

$$\tau_{cr}/G=\omega a \ln(d'/a)/2\pi(1-\nu)d' \quad (4)$$

where a is the starting migration distance. As has been noted in a review article [4], for tilt angles in the range of $5°<\omega<30°$ and for grain sizes in the range of 10–30 nm, formula (4) gives τ_{cr} in the range 20–300 MPa, well in the prevailing range of stress level for many fcc metals with grain sizes in that range. Also, recently, stress-driven migration of GBs has been described as a toughening micromechanism in nanocrystalline materials [42, 44].

This role is indirectly supported by the experimental observations [37] of the athermal grain growth in the vicinities of cracks in nanocrystalline materials.

Partial dislocations that carry partial dislocation slip and twin deformation have been experimentally observed in nanocrystalline metals (see, e.g., [12, 45–51]) (Figure 5). In particular, pairs of partial dislocations emitted from grain boundaries and connected by wide stacking faults have been experimentally observed in nanocrystalline Al [48], despite the fact that their formation in coarse-grained Al is commonly hampered due to high values of the specific stacking fault energy. These experiments are indicative of the strong nanoscale and interface effects that enhance the partial dislocation slip. Also, twin deformation has been experimentally observed in nanocrystalline metals such as Al, Cu, Ni, and Ta (for a review, see [51]). Deformation twinning in these materials is sensitive to the stacking fault energy, but the grain size also affects this process. In addition to the twin deformation carried by partial dislocations emitted from the grain boundaries, nanoscale twins can be generated through nanoscale multiplane ideal shear in deformed nanocrystalline solids and metal nanowires [52]. Twin deformation plays an important role, in particular, in nanocrystalline metals deformed at high strain rates and low temperatures, in which case, intergrain sliding and grain boundary diffusion are suppressed.

Also, there are situations where lattice dislocations effectively carry plastic deformation in even nanocrystalline metallic materials with finest grains, but not only those with intermediate grains. In particular, these situations are related to deformation under very high stresses, which, in particular, come into play in local regions near crack tips and specimens under shock load. For instance, lattice dislocations were experimentally observed within nanograins of nanocrystalline Ni after laser-induced shock load [53] and in vicinities of crack tips in quasi-statically deformed nanocrystalline Pt [54]. In the former case, high densities of lattice dislocations can be effectively produced by the generation and evolution of nanodisturbances (nanoscale areas where ideal plastic shear occurs) [55, 56]. The generation of lattice dislocations near crack tips can occur at both crack-free surfaces and nearest grain boundaries under high stress action [57].

5 Concluding remarks

Thus, with the specific structural features of nanocrystalline materials, the set of deformation mechanisms in these materials is richer than that in conventional coarse-grained polycrystals. In particular, in parallel with conventional lattice slip and twin deformation, such deformation mechanisms as intergrain sliding, grain boundary diffusional creep, triple junction diffusional creep, stress-driven migration of grain boundaries, rotational, and nanodisturbance deformation modes effectively operate in nanocrystalline metallic materials. Grain boundary deformation mechanisms dominate in nanocrystalline metallic materials with the finest grains (with grain size $d<d_c$). Plastic deformation through lattice dislocation slip is typically dominant in nanocrystalline metals having intermediate grains (with grain size being in the range $d_c<d<100$ nm). In doing so, the lattice slip is controlled by grain boundaries serving as effective stoppers, sources,

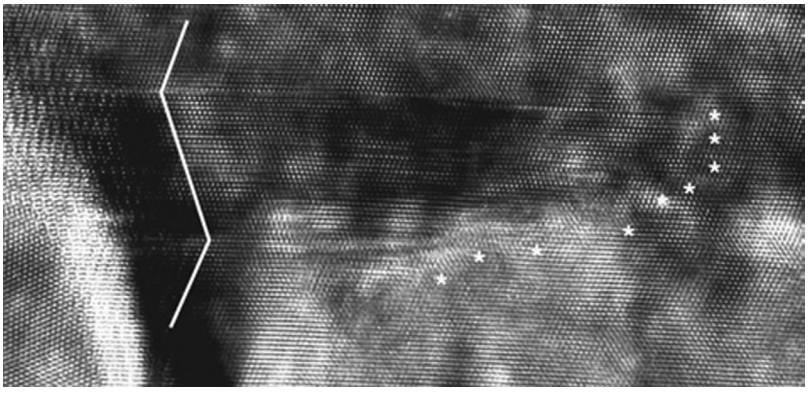

Figure 5 A high-resolution transmission electron microscopy image of a twin formed by plastically deforming electrodeposited nanocrystalline Ni.
The twin was formed by the emission of partials from grain boundary on the left, and it ended in the grain interior as marked by the white asterisks. Reprinted from [50]. Copyright 2009, with permission from the American Institute of Physics.

and sinks of perfect and partial lattice dislocations. Partial dislocations emitted from the grain boundaries also serve as carriers of nanoscale twin deformation, which occurs in nanocrystalline metals with widely ranged grain sizes. Nanodisturbance deformation mode comes into play in such metals at very high stresses.

The deformation mechanisms in nanocrystalline metallic materials are typically characterized by both low strain hardening and very high flow stresses close to the stress level needed to initiate cracks [1–7]. As a consequence of these factors, nanocrystalline metals commonly show low tensile ductility [1–7, 11]. At the same time, there are several examples of superstrong nanocrystalline metallic materials exhibiting a good tensile ductility (see [1–7, 11] and references therein). Systematic achievement of simultaneously high strength and good tensile ductility in nanocrystalline metallic materials at widely ranged conditions (chemical compositions, structural parameters, conditions of mechanical load) represents a very important unresolved problem in nanomaterials science. This problem is of large significance for development of structural applications of nanocrystalline materials. In the context discussed, further experimental identification, computer modeling, and theoretical description of deformation mechanisms and their mutual interactions (enhancing their cooperative actions) in nanocrystalline metals are of crucial importance for scientific and technological progress in this area.

Acknowledgments: The work was supported, in part, by the Russian Ministry of Science and Education (contract 14.740.11.0353).

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